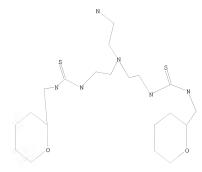
= 3

Uploading C:\Documents and Settings\jlau1\My Documents\10580856 - CD dimer\generic base structure.str

### L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s 11 sss sam

SAMPLE SEARCH INITIATED 09:48:13 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE
```

100.0% PROCESSED 3 ITERATIONS SEARCH TIME: 00.00.02 3 ANSWERS

L2 3 SEA SSS SAM L1

=> d 12 scan

L2 3 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Thiourea, 6',6''...'..'[nitrilotris(2,1-ethanediyliminocarbonothioylimino)]tris(N-[(3-methyl-3H-diazirin-3-yl)methyl]-N'-(2,3,4-tri-0-acetyl-6-deoxy-a-D-mannopyranosyl) (9CI)

MF C57 H87 N19 O21 S6

PAGE 1-B

```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1
    3 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
TN
    B-Cyclodextrin, 6A,6'A-[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethy
    1]imino]bis(2,1-ethanediyliminocarbonothioylimino)]bis[6A-deoxy- (9CI)
MF
    C97 H164 N6 O70 S2
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1
L2
    3 ANSWERS
               REGISTRY COPYRIGHT 2008 ACS on STN
IN
    B-Cyclodextrin, 6A, 6'A-[[[2-[[[2-(\alpha-D-mannopyranosyloxy)-1,1-
     bis[(\alpha-D-mannopyranosyloxy)methyl]ethyl]amino]thioxomethyl]amino]eth
     yl]imino]bis(2,1-ethanediyliminocarbonothioylimino)]bis[6A-deoxy- (9CI)
MF
    C115 H195 N7 O86 S3
CT
    COM
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
ALL ANSWERS HAVE BEEN SCANNED
=> s 11 sss full
FULL SEARCH INITIATED 09:48:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -
                                    47 TO ITERATE
100.0% PROCESSED
                      47 ITERATIONS
                                                                18 ANSWERS
SEARCH TIME: 00.00.01
T. 3
            18 SEA SSS FUL L1
=> d 13 1-18
L3
    ANSWER 1 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
RN
    888323-14-6 REGISTRY
ED
    Entered STN: 19 Jun 2006
```

Thiourea, 6'',6'''',6'''''-[nitrilotris(2,1-ethanedivliminocarbonothiovli mino)]tris[N-(6-deoxy-\alpha-D-mannopyranosy1)-N'-[(3-methy1-3H-diazirin-

STEREOSEARCH MF C39 H69 N19 O12 S6

FS

3-yl)methyl]- (9CI) (CA INDEX NAME)

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry. Rotation (+).

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L3 ANSWER 2 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 888323-13-5 REGISTRY
- ED Entered STN: 19 Jun 2006
- CN Thiourea, 6'',6'''',6'''''-[nitrilotris(2,1-ethanediyliminocarbonothioylimino)]tris[N-[(3-methyl-3H-diazirin-3-yl)methyl]-N'-(2,3,4-tri-0-acetyl-6-deoxy-c-D-mannopyranosyl)- (9C1) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C57 H87 N19 O21 S6
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry. Rotation (+).

PAGE 1-B

PAGE 2-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L3 ANSWER 3 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 851959-64-3 REGISTRY
- ED Entered STN: 09 Jun 2005
- CN  $\beta$ -Cyclodextrin,  $6A, 6^1A-[[[2-[([1/2-(\alpha-D-mannopyranosyloxy)-1, 1-bis[(\alpha-D-mannopyranosyloxy)methyl]ethyl]amino]thioxomethyl]amino]bis[(2,1-ethanediyliminocarbonothioylimino)]bis[6A-deoxy-, compd. with (2aR, 48, 4aS, 6R, 98, 118, 128, 12aR, 12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a, 3, 4, 4a, 5, 6, 9, 10, 11, 12, 12a, 12b-dodecahydro-4, 6, 11-trihydroxy-4a, 8, 13, 13-tetramethyl-5-oxo-7, 11-methano-1H-cyclodeca[3, 4]benz[1, 2-b]oxet-9-yl(\alphaR, <math>\beta$ S)- $\beta$ -[[[(1,1-dimethylethoxy)carbonyl]amino]- $\alpha$ -hydroxybenzenepropanoate (1:1) (9C1) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C115 H195 N7 O86 S3 . C43 H53 N O14
- SR
- LC STN Files: CA, CAPLUS, USPATFULL

CM

CRN 851959-57-4 CMF C115 H195 N7 O86 S3

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

CM

2

CRN 114977-28-5 CMF C43 H53 N O14

Absolute stereochemistry. Rotation (-).

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L3 ANSWER 4 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 851959-63-2 REGISTRY
- Entered STN: 09 Jun 2005 ED
- CN β-Cyclodextrin, 6A,6'A-[[[2-[[(methylamino)thioxomethyl]amino]ethyl]i mino|bis(2,1-ethanediyliminocarbonothioylimino)|bis[6A-deoxy-, compd. with (2aR, 4S, 4aS, 6R, 9S, 11S, 12S, 12aR, 12bS) -12b-(acetyloxy) -12-(benzoyloxy)-2a, 3, 4, 4a, 5, 6, 9, 10, 11, 12, 12a, 12b-dodecahydro-4, 6, 11-trihydroxy-4a, 8, 13, 13tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-v1  $(\alpha R, \beta S) - \beta - [[(1, 1-dimethylethoxy)carbonyl]amino] - \alpha$ hydroxybenzenepropanoate (1:1) (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C94 H159 N7 O68 S3 . C43 H53 N O14
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

CM

CRN 851959-52-9

CMF C94 H159 N7 O68 S3

PAGE 2-A

но-сн2

PAGE 3-A

PAGE 4-A

$$\begin{array}{c} & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

CM 2

CRN 114977-28-5 CMF C43 H53 N 014

Absolute stereochemistry. Rotation (-).

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L3 ANSWER 5 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 851959-60-9 REGISTRY
- ED Entered STN: 09 Jun 2005
- CN β-Cyclodextrin, 6A,6'A-[[[12-(α-D-mannopyranosylamino)-8-[2-
  - [[( $\alpha$ -D-mannopyranosylamino)thioxomethyl]amino]ethyl]-4,12-dithioxo-3,5,8,11-tetraazadodec-1-yl]imino]bis(2,1-ethanediyliminocarbonothioylimino)bis(6,A-deoxv-(9C1) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C113 H194 N12 O78 S5
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

PAGE 1-A





PAGE 4-A

но-

но-

но

## \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1907 TO DATE)
  1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 6 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN

- RN 851959-57-4 REGISTRY
- ED Entered STN: 09 Jun 2005
- CN β-Cyclodextrin, 6A,6'A-[[[2-[[[2-(α-D-mannopyranosyloxy)-1,1-bis](α-D-mannopyranosyloxy)methyl]ethyl]amino]thioxomethyl]amino]eth yl]imino]bis(2,1-ethanediyliminocarbonothioylimino)]bis[6A-deoxy-(9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C115 H195 N7 O86 S3
  - I COM
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL
- \*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*
- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
  - 1 REFERENCES IN FILE CA (1907 TO DATE)
- L3 ANSWER 7 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 851959-56-3 REGISTRY
- ED Entered STN: 09 Jun 2005
- CN  $\beta$ -Cyclodextrin, 6A,6'A-[[[2-[[[2-[(2,3,4,6-tetra-O-acetyl- $\alpha$ -D-mannopyranosyl)oxy]-1,1-bis[[(2,3,4,6-tetra-O-acetyl- $\alpha$ -D-

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- mannopyranosyl)oxy]methyl]ethyl]amino]thioxomethyl]amino]ethyl]imino]bis(2
  ,1-ethanediyliminocarbonothioylimino)]bis[6A-deoxy- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C139 H219 N7 O98 S3
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL
- \*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*
- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
  - 1 REFERENCES IN FILE CA (1907 TO DATE)
    1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 8 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 851959-55-2 REGISTRY
- ED Entered STN: 09 Jun 2005
- CN  $\beta$ -Cyclodextrin, 6A,6'A-[[[2-[[( $\alpha$ -D
  - mannopyranosylamino)thioxomethyl]amino]ethyl]imino]bis(2,1ethanediyliminocarbonothioylimino)]bis[6A-deoxy- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C99 H167 N7 O73 S3
- SR

CA

- LC STN Files: CA, CAPLUS, USPATFULL
- \*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*
- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
  - - 1 REFERENCES IN FILE CA (1907 TO DATE)
      1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 9 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 851959-54-1 REGISTRY

- ED Entered STN: 09 Jun 2005
- CN β-Cyclodextrin, 6A,6'A-[[[2-[[(2,3,4,6-tetra-0-acetyl-α-D-mannopyranosyl)amino]thioxomethyl]amino]ethyl]amino]thioxomethyl]amino]ethyl]amino]thioxomethyl]amin
- FS STEREOSEARCH
- MF C107 H175 N7 O77 S3
- SR

CA

- LC STN Files: CA, CAPLUS, USPATFULL
- \*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*
- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
  - 1 REFERENCES IN FILE CA (1907 TO DATE)
    1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 10 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 851959-53-0 REGISTRY
- ED Entered STN: 09 Jun 2005
- CN β-Cyclodextrin, 6A,6'A-[[[2-[[(phenylamino)thioxomethyl]amino]ethyl]i mino]bis(2,1-ethanediyliminocarbonothioylimino)]bis[6A-deoxy- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH

CA

- MF C99 H161 N7 O68 S3
- SR
- LC STN Files: CA, CAPLUS, USPATFULL

PAGE 1-A

## PAGE 4-A

$$\begin{array}{c} & & & & \\ & & & & \\ &$$

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L3 ANSWER 11 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 851959-52-9 REGISTRY
- ED Entered STN: 09 Jun 2005
- CN β-Cyclodextrin, 6A,6'A-[[[2-[[(methylamino)thioxomethyl]amino]ethyl]i mino]bis(2,1-ethanediyliminocarbonothioylimino)]bis[6A-deoxy- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C94 H159 N7 O68 S3
- CI COM
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

PAGE 2-A

но-сн2

PAGE 4-A

R2

$$\begin{array}{c} & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ &$$

HO-CH<sub>2</sub>

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

# 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L3 ANSWER 12 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 765963-63-1 REGISTRY
- ED Entered STN: 20 Oct 2004
- CN  $\beta$ -Cyclodextrin, 6A,6'A-[[(2-aminoethyl)imino]bis(2,1-

ethanediyliminocarbonothioylimino)]bis[6A-deoxy- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C92 H156 N6 O68 S2

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

PAGE 1-A

PAGE 2-A

но-сн2

PAGE 4-A

HO-CH<sub>2</sub>

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 13 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 765963-62-0 REGISTRY
- ED Entered STN: 20 Oct 2004
- CN β-Cyclodextrin, 6A,6'a-[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethy limino]bis (2,1-ethanediyliminocarbonothioylimino)]bis [6A-deoxy- (9CI) (CA INDEX NAME)

```
FS
     STEREOSEARCH
     CA
```

ME C97 H164 N6 O70 S2

SR

LC CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL STN Files:

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 14 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN L3

RN 765963-60-8 REGISTRY

ED Entered STN: 20 Oct 2004

CN  $\alpha$ -D-Glucopyranoside, 6,6'-[[[15-( $\alpha$ -D-mannopyranosyloxy)-8-[2-[[[2-( $\alpha$ -D-mannopyranosyloxy)-1,1-bis[( $\alpha$ -D-

mannopyranosyloxy)methyl]ethyl]amino]thioxomethyl]amino]ethyl]-14,14bis  $[(\alpha-D-mannopyranosyloxy)methyl]-4,12-dithioxo-3,5,8,11,13$ pentaazapentadec-1-v1|imino|bis(2,1-ethanedivliminocarbonothiovlimino)|bis [methyl 6-deoxy- (9CI) (CA INDEX NAME)

STEREOSEARCH FS

ME C75 H138 N12 O46 S5

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L3 ANSWER 15 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 211985-74-9 REGISTRY
- ED Entered STN: 01 Oct 1998

- CN q-D-Mannopyranoside, 6,6',6''-[nitrilotris(2,1-ethanediyliminocarbonothioylimino)]tris[4-nitrophenyl 6-deoxy- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C45 H60 N10 O21 S3
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (+).

PAGE 2-A

PAGE 2-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 16 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN RN -211985-73-8 REGISTRY

- ED Entered STN: 01 Oct 1998
- CN α-D-Mannopyranoside, 6,6',6''-[nitrilotris(2,1ethanediyliminocarbonothioylimino)]tris[methyl 6-deoxy- (9CI) (CA INDEX NAME)
- STEREOSEARCH CA
- C30 H57 N7 O15 S3 MF
- SR
- LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (+).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 17 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN L3
- RN 211985-72-7 REGISTRY
- ED Entered STN: 01 Oct 1998
- CN α-D-Mannopyranoside, 6,6',6''-[nitrilotris(2,1ethanediyliminocarbonothioylimino)]tris[methyl 6-deoxy-, 2,2',2'',3,3',3'',4,4',4''-nonaacetate (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C48 H75 N7 O24 S3
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (+).

PAGE 1-B

- OAc

OAc

L3

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

# 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 18 OF 18 REGISTRY COPYRIGHT 2008 ACS on STN

- RN 211985-71-6 REGISTRY
- ED Entered STN: 01 Oct 1998
- CN  $\alpha$ -D-Mannopyranoside, 6,6',6''-[nitrilotris(2,1-ethanediyliminocarbonothioylimino)]tris[methyl 6-deoxy-,
  - 2,2',2'',3,3',3'',4,4',4''-nonabenzoate (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C93 H93 N7 O24 S3
- SR CA
- LC STN Files: CA, CAPLUS

PAGE 1-B

PAGE 2-B

Ph

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 214.82 215.03

FULL ESTIMATED COST

=> b caplus

FILE 'CAPLUS' ENTERED AT 09:49:17 ON 16 JUL 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 16 Jul 2008 VOL 149 ISS 3 FILE LAST UPDATED: 15 Jul 2008 (20080715/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s 13 L4 4 L3

=> s 14 and py<=2003 23986215 PY<=2003 GT

=> d 15 ibib abs

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:433682 CAPLUS <<LOGINID::20080716>>

DOCUMENT NUMBER: 129:203149

ORIGINAL REFERENCE NO.: 129:41271a,41274a

TITLE: Multivalent ligands for the mannose-specific lectin on

type 1 fimbriae of Escherichia coli : syntheses and

testing of trivalent α-D-mannoside clusters AUTHOR(S):

Kotter, Sven; Krallmann-Wenzel, Ulrike; Ehlers,

Stefan; Lindhorst, Thisbe K.

CORPORATE SOURCE: Department of Organic Chemistry, University of

Hamburg, Hamburg, D-20146, Germany

SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1998),

(14), 2193-2200

CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Roval Society of Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

AB The syntheses of the tri-antennary cluster  $\alpha$ -D-mannosides 16, 19, 23 and 24 and their capacities to inhibit mannose-dependent binding of E. coli HB 101 (pPK14) are described. The cluster glycosides are formed by glycosylation of tris-(3-hydroxypropyl)nitromethane, by linking of suitable mannoside derivs. via amide and thiourea bonds to tris-(2-carboxyethyl)nitromethane and tris-(2-aminoethyl)amine. Functionalized mannosides are attached to the core mols. at the 6-position of the sugar ring to allow variation of the introduced aglycon moieties in order to compare their effects on the inhibitory potencies of the derived mannoside clusters. The 6-peptide-bridged cluster mannoside (I) displays the highest binding potency towards the type 1 fimbrial lectin of E. coli as tested by inhibition agglutination tests and ELISA.

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 14 scan

4 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN

63-6 (Pharmaceuticals)

Section cross-reference(s): 35

- TI Optimizing saccharide-directed molecular delivery to biological receptors: design, synthesis, and biological evaluation of glycodendrimercvclodextrin conjugates
- ST glycodendrimer cyclodextrin conjugate Taxotere lectin Con A binding

IT Dendritic polymers

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(conjugates with cyclodextrin; design and synthesis and biol. evaluation of glycodendrimer-cyclodextrin conjugates for molecularly directed delivery of docetaxel)

IT Macrophage

(design and synthesis and biol. evaluation of glycodendrimer-cyclodextrin conjugates for molecularly directed delivery of docetaxel)

IT Agglutinins and Lectins

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(design and synthesis and biol. evaluation of glycodendrimer-

cyclodextrin conjugates for molecularly directed delivery of docetaxel)

IT Drug delivery systems

(prodrugs; design and synthesis and biol. evaluation of glycodendrimer-cyclodextrin conjugates for molecularly directed delivery of docetaxel)

IT 11028-71-0, Con A

ΙT

RI: BSU (Biological study, unclassified); BIOL (Biological study) (binding with dendritic cyclodextrin conjugates; design and synthesis and biol. evaluation of glycodendrimer-cyclodextrin conjugates for molecularly directed delivery of docetaxel)

II 250329-55-6P 307980-95-6P 307980-97-8P 307980-99-0P 307981-01-7P 307981-03-9P 30981-01-7P 307981-03-9P 30943-03-9P 765963-59-6P 765963-55-6P 765963-55-7P 765963-55-3P 765963-55-1P 765963-55-1P 765963-55-2P 765963-57-3P 765963-58-4P 765963-59-5P 765963-68-6P 765963-59-5P 765963-68-6P 7659

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation), USES (Uses)

(design and synthesis and biol. evaluation of glycodendrimercyclodextrin conjugates for molecularly directed delivery of docetaxel)
114977-28-5, (Taxotere)

RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(design and synthesis and biol. evaluation of glycodendrimercyclodextrin conjugates for molecularly directed delivery of docetaxel) 849832-26-4P

RL: CRT (Combinatorial reactant); RCT (Reactant); SPN (Synthetic preparation); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent)

(design and synthesis and biol. evaluation of glycodendrimer-cyclodextrin conjugates for molecularly directed delivery of docetaxel)

IT 765963-67-5P 766549-80-8P RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(design and synthesis and biol. evaluation of glycodendrimercyclodextrin conjugates for molecularly directed delivery of docetaxel)

IT 80-40-0 111-40-0 463-71-8, Thiophosgene 4097-89-6 5155-47-5, Methyl 6-amino-6-deoxy-α-D-glucopyranoside 5515-02-6 29390-67-8 58632-95-4 93221-21-7 149876-86-8 207347-75-9 765963-61-9 765963-64-2

```
RL: RCT (Reactant); RACT (Reactant or reagent)
        (design and synthesis and biol. evaluation of glycodendrimer-
        cyclodextrin conjugates for molecularly directed delivery of docetaxel)
     117499-16-8P 179167-09-0P 250329-52-3P 307980-79-6P 307980-81-0P
     307980-83-2P 307980-85-4P 307980-87-6P 307980-89-8P 307980-91-2P
     307980-93-4P 765963-43-7P 765963-44-8P 765963-45-9P 765963-46-0P
     765963-47-1P 765963-48-2P <u>765963-62-0P 765963-63-1P</u>
765963-65-3P 765963-66-4P <u>849832-16-2P 849832-17-3P</u>
                                                                  849832-18-4P
     849832-27-5P 849832-28-6P 849834-36-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (design and synthesis and biol. evaluation of glycodendrimer-
        cyclodextrin conjugates for molecularly directed delivery of docetaxel)
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1
L4
      4 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
     ICM C08B037-16
     ICS A61K047-48; A61K031-337; A61P035-00
     33-4 (Carbohydrates)
     Section cross-reference(s): 6, 63
TТ
    New cyclodextrin dimers and their derivatives, their preparation
     processes, and their use in particular for solubilization of
     pharmacologically active substances
ST
    cyclodextrin dimer prepn solubilization pharmacol Con A inclusion taxotere
IT
    Oligosaccharides, preparation
     RL: BSU (Biological study, unclassified); IMF (Industrial manufacture);
     SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
        (cyclic; process Preparation of cyclodextrin dimers and their use for
        solubilization of pharmacol, active substances)
ΙT
    Solubilization
        (process Preparation of cyclodextrin dimers and their use for solubilization
        of pharmacol. active substances)
     Inclusion compounds
     RL: BSU (Biological study, unclassified); IMF (Industrial manufacture);
     SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
        (process preparation of cyclodextrin dimers and their use for solubilization
        of pharmacol, active substances)
ΤТ
     11028-71-0, ConA
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (process preparation of cyclodextrin dimers and their use for solubilization
        of pharmacol. active substances)
     766549-80-8P 851959-63-2P 851959-64-3P
     RL: BSU (Biological study, unclassified); IMF (Industrial manufacture);
     BIOL (Biological study); PREP (Preparation)
        (process preparation of cyclodextrin dimers and their use for solubilization
        of pharmacol. active substances)
     766549-42-2P 851959-54-1P 851959-55-2P
     851959-57-4P 851959-60-9P
     RL: BSU (Biological study, unclassified); IMF (Industrial manufacture);
     SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
        (process preparation of cyclodextrin dimers and their use for solubilization
        of pharmacol. active substances)
    113738-22-0P 117499-16-8P
                                  179167-09-0P 765963-61-9P
     765963-62-0P 765963-63-1P 765963-64-2P 849834-36-2P
     \frac{851959-52-9P}{851959-58-5P} \frac{851959-53-0P}{851959-59-6P} \frac{851959-56-3P}{851959-61-0P} \frac{851959-62-1P}{851959-62-1P}
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
```

preparation); PREP (Preparation); RACT (Reactant or reagent)

(process preparation of cyclodextrin dimers and their use for solubilization of pharmacol. active substances)

- 103-71-9, Phenvl isocvanate, reactions 111-40-0, Diethylenetriamine 463-71-8, Thiophosgene 540-51-2, 2-Bromoethanol 624-83-9, Methyl isocyanate 4097-89-6 29390-67-8 58632-95-4 93221-21-7 307980-79-6
  - RL: RCT (Reactant); RACT (Reactant or reagent)

(process preparation of cyclodextrin dimers and their use for solubilization of pharmacol, active substances)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- T. 4 4 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- CC 33-7 (Carbohydrates)
  - Section cross-reference(s): 10
- ΤТ A modular system for the preparation of diazirine-labeled mannose
- derivatives using thiourea bridging ST thiourea azirine mannose glycoside prepn Escherichia coli
- ΙT

Escherichia coli (synthesis of photolabile diazirine-labeled mannosides and mannosyl

- clusters) Aminoglycosides
- RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
- (synthesis of photolabile diazirine-labeled mannosides and mannosyl clusters)
- 78-96-6 93221-21-7 150771-92-9 182347-32-6 222990-01-4 888323-08-8
  - RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis of photolabile diazirine-labeled mannosides and mannosyl clusters)

- 170384-29-9P 882516-43-0P 882516-45-2P 888323-01-1P 888323-02-2P 888323-03-3P 888323-04-4P 888323-06-6P 888323-09-9P 888323-11-3P
  - 888323-12-4P 888323-13-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
  - (synthesis of photolabile diazirine-labeled mannosides and mannosyl clusters)
- IΤ 4097-89-6P 882516-53-2P 888323-05-5P 888323-07-7P 888323-10-2P 888323-14-6P
  - RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of photolabile diazirine-labeled mannosides and mannosyl clusters)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 4 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN L4
- CC 33-3 (Carbohydrates)
  - Section cross-reference(s): 1, 6
- Multivalent ligands for the mannose-specific lectin on type 1 fimbriae of Escherichia coli : syntheses and testing of trivalent a-D-mannoside clusters
- mannoside cluster binding inhibition Escherichia prepn
- Escherichia coli

(syntheses of trivalent  $\alpha$ -D-mannoside clusters as multivalent ligands for the mannose-specific lectin on type 1 fimbriae of Escherichia coli)

```
Dendritic polymers
    Glycosides
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (syntheses of trivalent \alpha-D-mannoside clusters as multivalent
        ligands for the mannose-specific lectin on type 1 fimbriae of
        Escherichia coli)
    10357-27-4
IT
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); BIOL (Biological study); RACT
     (Reactant or reagent)
        (syntheses of trivalent a-D-mannoside clusters as multivalent
        ligands for the mannose-specific lectin on type 1 fimbriae of
        Escherichia coli)
    211985-68-1P 211985-70-5P \underline{211985-73-8P} \underline{211985-74-9P} RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (syntheses of trivalent \alpha\text{-D-mannoside} clusters as multivalent
        ligands for the mannose-specific lectin on type 1 fimbriae of
        Escherichia coli)
     4097-89-6 59085-15-3 83441-60-5 92528-09-1
                                                           116747-80-9
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (syntheses of trivalent \alpha-D-mannoside clusters as multivalent
        ligands for the mannose-specific lectin on type 1 fimbriae of
        Escherichia coli)
```

IT 18439-61-7P 66224-56-4P 79695-15-1P 150771-91-8P 150771-92-9P 211985-62-5P 211985-63-6P 211985-64-7P 211985-65-8P 211985-66-9P 211985-67-0P 211985-67-0P 211985-67-0P 211985-71-6P 211985-72-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(syntheses of trivalent  $\alpha\text{-D-mannoside}$  clusters as multivalent ligands for the mannose-specific lectin on type 1 fimbriae of Escherichia coli)

ALL ANSWERS HAVE BEEN SCANNED

STR

```
=> d his

(FILE 'HOME' ENTERED AT 09:47:31 ON 16 JUL 2008)

FILE 'REGISTRY' ENTERED AT 09:47:51 ON 16 JUL 2008

L1 STRUCTURE UPLOADED

L2 3 S L1 SSS SAM

L3 18 S L1 SSS FULL

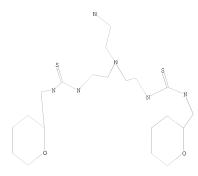
FILE 'CAPLUS' ENTERED AT 09:49:17 ON 16 JUL 2008

L4 4 S L3

L5 1 S L4 AND PY<=2003

=> d 11

L1 HAS NO ANSWERS
```



Structure attributes must be viewed using STN Express query preparation.

=> logoff hold COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.99	221.02
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL
CA SUBSCRIBER PRICE	-0.80	-0.80

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 09:50:26 ON 16 JUL 2008